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PASSWORD:

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CAS World Wide Web Site (general information)

FILE 'HOME' ENTERED AT 14:21:56 ON 15 MAY 2002

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL

NEWS WWW

ENTRY SESSION FULL ESTIMATED COST 0.21

0.21

FILE 'REGISTRY' ENTERED AT 14:22:06 ON 15 MAY 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 13 MAY 2002 HIGHEST RN 415678-09-0 DICTIONARY FILE UPDATES: 13 MAY 2002 HIGHEST RN 415678-09-0

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

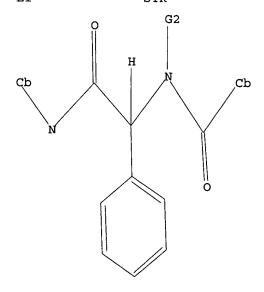
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

Uploading 09852965-3.str

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS T.1 STR



G1 G2 Cy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

09/852,965

SAMPLE SEARCH INITIATED 14:22:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1673 TO ITERATE

59.8% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01 0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 31007 TO 35913 PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss ful FULL SEARCH INITIATED 14:22:53 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 32586 TO ITERATE

100.0% PROCESSED 32586 ITERATIONS 27 ANSWERS SEARCH TIME: 00.00.04

L3 27 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
140.66
140.87

FILE 'CAPLUS' ENTERED AT 14:23:04 ON 15 MAY 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 15 May 2002 VOL 136 ISS 20 FILE LAST UPDATED: 13 May 2002 (20020513/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s 13 L4 13 L3

=> d 14 1-13 bib hitstr

```
ANSWER 1 OF 13 CAPLUS COPYRIGHT 2002 ACS
L4
AN
       2001:453049 CAPLUS
DN
       135:45999
       Synthesis and use of serine protease inhibitors (substituted phenylglycine
ΤI
       derivatives) as antiinflammatory agents
       Lively, Sarah Elizabeth; Waszkowycz, Bohdan; Harrison, Martin James;
IN
       Farthing, Christopher Neil; Johnson, Keith Michael
       Protherics Molecular Design Limited, UK
PA
       PCT Int. Appl., 171 pp.
so
       CODEN: PIXXD2
DT
       Patent
       English
LA
FAN.CNT 11
                                                                 APPLICATION NO. DATE
       PATENT NO.
                                 KIND DATE
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                                           20010621
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       WO 2000077027
                                  A2
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       WO 2000077027
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        WO 2001096305
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                                                                WO 2001-GB2566 20010612
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PRAI GB 1999-29552
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                                           19991214
        WO 2000-GB2291
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       US 1999-142064P
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                                           19990702
       GB 1999-18741
                                   Α
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       GB 1999-29553
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        WO 2000-GB4764
                                   W
                                           20001213
os
       MARPAT 135:45999
IT
        344933-13-7P 344933-14-8P 344933-15-9P
        RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
        (Reactant or reagent)
             (synthesis and use of (hetero) arom. substituted phenylglycine derivs.
            as antiinflammatory agents)
RN
        344933-13-7 CAPLUS
```

Carbamic acid, [[3-[[2-[(2,3-dihydro-1H-inden-5-yl)amino]-1-(4-CN methylphenyl) -2-oxoethyl] [(2,4-dimethoxyphenyl) methyl] amino] carbonyl] pheny l]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN

344933-14-8 CAPLUS Benzoic acid, 4-[2-[(2,3-dihydro-1H-inden-5-yl)amino]-1-[[(2,4-CN dimethoxyphenyl) methyl] [3-[[[(1,1-dimethylethoxy) carbonyl] amino] methyl] ben
zoyl] amino] -2-oxoethyl] -, methyl ester (9CI) (CA INDEX NAME)

RN

344933-15-9 CAPLUS
Benzoic acid, 4-[2-[(2,3-dihydro-1H-inden-5-yl)amino]-1-[[(2,4-CN dimethoxyphenyl) methyl] [3-[[[(1,1-dimethylethoxy)carbonyl]amino]methyl]ben zoyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 2 OF 13 CAPLUS COPYRIGHT 2002 ACS
L4
      2001:167962 CAPLUS
AN
      134:222529
DN
      Preparation of aromatic trifluoromethylsulfonyl and
TI
      trifluoromethylsulfonamido compounds as phosphate mimics and phosphatase
      inhibitors and methods of treatment
      Huang, Ping; Wei, Chung Chen; Tang, Peng Cho; Liang, Chris; Ramphal, John;
IN
      Jallal, Bahija; Blitz, John; Li, Sharon; Mattson, Matthew Neil; Mcahon,
      Gerald; Koenig, Marcel
PΑ
      Sugen, Inc., USA; et al.
      PCT Int. Appl., 262 pp.
SO
      CODEN: PIXXD2
DT
      Patent
LA
      English
FAN.CNT 1
      PATENT NO.
                              KIND DATE
                                                           APPLICATION NO. DATE
                                      20010308
                                                           WO 2000-US23293 20000825
PΊ
      WO 2001016097
                              A1
            W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                             P
PRAI US 1999-150970P
                                      19990827
      US 1999-165365P
                               Р
                                      19991112
os
      MARPAT 134:222529
      329317-75-1P, N-Cyclohexyl-N-[(2,6-dimethylphenylcarbamoyl)-(4-
      trifluoromethanesulfonylphenyl)methyl]benzamide
      RL: BAC (Biological activity or effector, except adverse); BSU (Biological
      study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
      BIOL (Biological study); PREP (Preparation); USES (Uses)
           (drug candidate; prepn. of arom. trifluoromethylsulfonyl and
           trifluoromethylsulfonamido compds. as phosphate mimics and phosphatase
           inhibitors)
```

RN 329317-75-1 CAPLUS

CN Benzeneacetamide, .alpha.-(benzoylcyclohexylamino)-N-(2,6-dimethylphenyl)-4-[(trifluoromethyl)sulfonyl]- (9CI) (CA INDEX NAME)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2002 ACS

AN 2001:50635 CAPLUS

DN 134:115845

TI Preparation of .alpha.,.beta.-annelated butyrolactones as modulators of metabotropic glutamate receptors.

IN Stolle, Andreas; Antonicek, Horst-Peter; Lensky, Stephan; Voerste, Arnd; Muller, Thomas; Baumgarten, Jorg; Von Dem Bruch, Karsten; Muller, Gerhard; Stropp, Udo; Horvath, Ervin; De Vry, Jean-Marie-Victor; Schreiber, Rudy

PA Bayer Aktiengesellschaft, Germany

SO PCT Int. Appl., 215 pp. CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

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PATENT NO.
                                             KIND
                                                         DATE
                                                                                         APPLICATION NO. DATE
                                              _ _ _ _
                                                          _____
                                                                                         _____
          WO 2001004107
                                               A1
                                                          20010118
                                                                                         WO 2000-EP6105
                                                                                                                             20000630
PΙ
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                  RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                                                                       DE 1999-19932621 19990713
          DE 19932621
                                               A1
                                                          20010426
PRAI DE 1999-19932621 A
                                                          19990713
          MARPAT 134:115845
OS
IT
          321128-05-6P
```

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of .alpha.,.beta.-annelated butyrolactones as modulators of metabotropic glutamate receptors)

RN 321128-05-6 CAPLUS

CN Benzeneacetamide, .alpha.-(benzoylmethylamino)-N-[4-[[(3aR,6aR)-tetrahydro-5-methylene-3-oxo-1H-cyclopenta[c]furan-3a(3H)-yl]methyl]phenyl]-, rel-

(9CI) (CA INDEX NAME)

Relative stereochemistry.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2002 ACS

AN 2000:454829 CAPLUS

DN 133:222996

TI Multicomponent synthesis of novel amino acid-nucleobase chimeras: a versatile approach to PNA-monomers

AU Maison, Wolfgang; Schlemminger, Imre; Westerhoff, Ole; Martens, Jurgen

CS Fachbereich Chemie, Universitat Oldenburg, Oldenburg, D-26111, Germany

SO Bioorganic & Medicinal Chemistry (2000), 8(6), 1343-1360 CODEN: BMECEP; ISSN: 0968-0896

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 133:222996

IT 292072-91-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(multicomponent synthesis of novel amino acid-nucleobase chimeras for use as PNA-monomers)

RN 292072-91-4 CAPLUS

CN Carbamic acid, [1-[[2-[[[2-(acetylamino)ethyl] [2-[[4-(1,1-dimethylethyl)-1-cyclohexen-1-yl]amino]-2-oxo-1-phenylethyl]amino]carbonyl]phenyl]methyl]1,2-dihydro-2-oxo-4-pyrimidinyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 70 ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 5 OF 13 CAPLUS COPYRIGHT 2002 ACS L4

2000:53602 CAPLUS AN

132:108299 DN

Preparation of precursors for PNA monomers TТ

Martens, Jurgen; Maison, Wolfgang; Schlemminger, Imre; Westerhoff, Ole; IN Groger, Harald

PA Germany

PCT Int. Appl., 72 pp. SO CODEN: PIXXD2

DT Patent

English LA

FAN.CNT 1

APPLICATION NO. DATE PATENT NO. KIND DATE _____ _ _ _ _ WO 1998-EP4281 19980710 PΙ WO 2000002864 A1 20000120 W: AT, AU, BG, BR, CA, CH, CN, CZ, DE, DK, ES, FI, GB, HR, HU, IL, JP, KR, LU, MK, MX, NO, NZ, PL, PT, RU, SE, SI, TR, US, YU
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG AU 1998-90645 AU 9890645 A1 20000201 19980710 PRAI WO 1998-EP4281 19980710

MARPAT 132:108299 OS

IT 255736-69-7P 255736-75-5P

> RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of precursors for PNA monomers)

255736-69-7 CAPLUS RN

Carbamic acid, [2-[[2-(1-cyclohexen-1-ylamino)-2-oxo-1-phenylethyl] [2-CN [(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)methyl]benzoyl]amino]et hyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

255736-75-5 CAPLUS RN

Benzeneacetamide, .alpha.-[[2-[(3,4-dihydro-2,4-dioxo-1(2H)-CN pyrimidinyl) methyl]benzoyl][2-[(2-methyl-1-oxopropyl)amino]phenyl]amino]-N-[4-(1,1-dimethylethyl)-1-cyclohexen-1-yl]- (9CI) (CA INDEX NAME)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2002 ACS
- AN 1999:662324 CAPLUS
- DN 132:64501
- TI Generation of an Ugi library of phosphate mimic-containing compounds and identification of novel dual specific phosphatase inhibitors
- AU Bergnes, Gustave; Gilliam, Carla L.; Boisclair, Michael D.; Blanchard, Jill L.; Blake, Katharine V.; Epstein, David M.; Pal, Kollol
- CS Department of Medicinal Chemistry, Mitotix, Inc., Cambridge, MA, 02139, USA
- SO Bioorganic & Medicinal Chemistry Letters (1999), 9(19), 2849-2854 CODEN: BMCLE8; ISSN: 0960-894X
- PB Elsevier Science Ltd.
- DT Journal
- LA English
- IT 253132-59-1P 253132-61-5P 253132-62-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(using the combinatorial Ugi reaction to prep. a library of dipeptidyl phosphate mimics to identify the binding requirements of Cdc25 phosphatase)

- RN 253132-59-1 CAPLUS
- CN Propanedioic acid, [4-[[(1,3-benzodioxol-5-ylmethyl)[2-(cyclohexylamino)-2oxo-1-[4-(phosphonomethoxy)phenyl]ethyl]amino]carbonyl]phenoxy]- (9CI)
 (CA INDEX NAME)

RN 253132-61-5 CAPLUS

CN Propanedioic acid, [4-[1-[(1,3-benzodioxol-5-ylmethyl)] [4-(phosphonomethyl)benzoyl]amino]-2-(cyclohexylamino)-2-oxoethyl]phenoxy]-(9CI) (CA INDEX NAME)

RN 253132-62-6 CAPLUS

CN Propanedioic acid, [4-[[(1,3-benzodioxol-5-ylmethyl) [2-(cyclohexylamino)-1-[4-(dicarboxymethoxy)phenyl]-2-oxoethyl]amino]carbonyl]phenoxy]- (9CI) (CA INDEX NAME)

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2002 ACS

AN 1999:45211 CAPLUS

DN 130:110408

TI Preparation of fluorous silicon, tin and germanium compounds and their use in organic synthesis to facilitate organic/fluorous extractive purification

Curran, Dennis P.; Hadida, Ruah Sabine; Hoshino, Masahide; Studer, Armido;
Wipf, Peter; Jeger, Patrick; Kim, Sun-young; Ferritto, Rafael

PA University of Pittsburgh, USA

SO U.S., 40 pp., Cont.-in-part of U.S. 5,777,121. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 2

	PATENT NO.														DATE			
					KIND		DATE			/ APPLICATION NO.				ο.				
ΡI	US 5859247				A A					U	US 1996-690491				19960731			
	US 5777121			-					US 1996-671945				19960628					
		-																
	ÇA	. 2259183			AA		19980108			CA 1997-2259183				199/0626				
	WO	9800376			A1		19980108			WO 1997-US11215				15	19970626			
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			GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,
			GN,	ML,	MR,	NE,	SN,	TD,	TG									
	ΑU	9735		Α	1	19980121			AU 1997-35818					19970626				
	EP	9076	25		Α	1	19990414			EP 1997-932333				3	19970626			
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	JΡ	2000	5140	62	T	2	20001024			J1	JP 1998-504319				19970626			

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20001205
                                         US 1998-80274
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    US 6156896
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PRAI US 1996-671945
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    WO 1997-US11215
                      W
                            19970626
    CASREACT 130:110408; MARPAT 130:110408
OS
    189077-35-8P
ΙT
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. from fluorous silylbenzoic acid, amine, aldehyde and isocyanide
       using org./fluorous extractive purifn.)
     189077-35-8 CAPLUS
RN
    Benzeneacetamide, .alpha.-[benzoyl(phenylmethyl)amino]-N-cyclohexyl- (9CI)
CN
       (CA INDEX NAME)
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RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

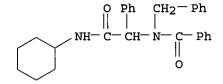
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ANSWER 8 OF 13 CAPLUS COPYRIGHT 2002 ACS
L4
AN
      1998:55597 CAPLUS
      128:127604
DN
      Fluorous reaction and separation systems
TΙ
      Curran, Dennis P.; Hadida, Ruah Sabine; Hashino, Masahide; Studer, Armido;
IN
      Wipf, Peter; Jeger, Patrick; Kim, Sun-young; Ferritto, Rafael
PA
      University of Pittsburgh, USA
      PCT Int. Appl., 120 pp.
SO
      CODEN: PIXXD2
DT
      Patent
      English
LA
FAN.CNT 2
                                                          APPLICATION NO. DATE
      PATENT NO.
                             KIND DATE
                             ----
                                      -----
                                                           -----
                                                          WO 1997-US11215 19970626
                                      19980108
PΤ
      WO 9800376
                              A1
           W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG
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      US 5777121
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                                      19980707
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      US 5859247
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                                                          AU 1997-35818
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                AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
                 IE, FI
      JP 2000514062
                                      20001024
                                                          JP 1998-504319
                                                                                19970626
                               T2
PRAI US 1996-671945
                               Α
                                      19960628
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                               Α
                                      19960731
      WO 1997-US11215
                               W
                                      19970626
OS
      CASREACT 128:127604; MARPAT 128:127604
TT
      189077-35-8P
```

RL: SPN (Synthetic preparation); PREP (Preparation) (fluorous reaction and sepn. systems)

RN 189077-35-8 CAPLUS

CN Benzeneacetamide, .alpha.-[benzoyl(phenylmethyl)amino]-N-cyclohexyl- (9CI) (CA INDEX NAME)





- L4 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2002 ACS
- AN 1997:253978 CAPLUS

DN 126:292891

TI Fluorous Synthesis: Fluorous Protocols for the Ugi and Biginelli Multicomponent Condensations

AU Studer, Armido; Jeger, Patrick; Wipf, Peter; Curran, Dennis P.

CS Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA

SO J. Org. Chem. (1997), 62(9), 2917-2924 CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

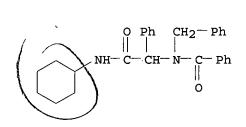
OS CASREACT 126:292891

IT 189077-35-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (application of fluorous protocols for Ugi and Biginelli multicomponent condensations)

RN 189077-35-8 CAPLUS

CN Benzeneacetamide, .alpha.-[benzoyl(phenylmethyl)amino]-N-cyclohexyl- (9CI) (CA INDEX NAME)





- L4 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2002 ACS
- AN 1996:133173 CAPLUS

DN 124:289157

TI Postcondensation Modifications of Ugi Four-Component Condensation Products: 1-Isocyanocyclohexene as a Convertible Isocyanide. Mechanism of Conversion, Synthesis of Diverse Structures, and Demonstration of Resin Capture

AU Keating, Thomas A.; Armstrong, Robert W.

CS Department of Chemistry and Biochemistry, University of California, Los Angeles, CA, 90095, USA

SO J. Am. Chem. Soc. (1996), 118(11), 2574-83 CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

IT 175606-32-3

RL: RCT (Reactant)

(modified of Ugi four-component condensation by use of isocyanatocyclohexene as isocyanide equiv.)

RN 175606-32-3 CAPLUS

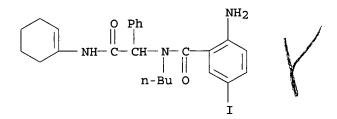
CN Benzeneacetamide, .alpha.-(benzoylbutylamino)-N-1-cyclohexen-1-yl- (9CI) (CA INDEX NAME)

IT 175606-23-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (modified of Ugi four-component condensation by use of isocyanocyclohexene as isocyanide equiv.)

RN 175606-23-2 CAPLUS

CN Benzeneacetamide, .alpha.-[(2-amino-5-iodobenzoyl)butylamino]-N-1-cyclohexen-1-yl- (9CI) (CA INDEX NAME)



L4 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2002 ACS

AN 1989:422724 CAPLUS

DN 111:22724

TI Organic syntheses via transition metal complexes. 35.
(C-Amino)keteneimines, 2-imidazolin-5-ones, and .alpha.-amino acids from aminocarbene chromium complexes and isocyanides

AU Aumann, Rudolf; Heinen, Heinrich

CS Org. Chem. Inst., Univ. Muenster, Muenster, D-4400, Fed. Rep. Ger.

SO Chem. Ber. (1989), 122(6), 1139-45 CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA German

OS CASREACT 111:22724

IT 119209-05-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 119209-05-1 CAPLUS

CN Benzeneacetamide, N-cyclohexyl-.alpha.-(dibenzoylamino)- (9CI) (CA INDEX

```
ANSWER 12 OF 13 CAPLUS COPYRIGHT 2002 ACS
L4
    1970:477105 CAPLUS
ΑN
DN
     73:77105
     Preparation and properties of mesoionic oxazolones
ΤI
     Bayer, Horst O.; Huisgen, Rolf; Knorr, Rudolf; Schaefer, Fred C.
AU
     Inst. Org. Chem., Univ. Muenchen, Munich, Ger.
CS
so
     Chem. Ber. (1970), 103(8), 2581-97
     CODEN: CHBEAM
DT
     Journal
     German
LA
     28544-59-4P
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
RN
     28544-59-4 CAPLUS
     Benzamide, N-methyl-N-[.alpha.-(p-tolylcarbamoyl)benzyl]- (8CI) (CA INDEX
CN
     NAME)
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ANSWER 13 OF 13 CAPLUS COPYRIGHT 2002 ACS
L4
ΑN
     1967:2461 CAPLUS
     66:2461
DN
     2,3,4,5-Tetrahydro-1H-3-benzazepin-1-ones and
ΤI
     hexahydroimidazoisoquinolines
ΑU
     Hazebroucq, Georges
     Pharm., Centrale Hop., Paris, Fr.
CS
     Ann. Chim. (Paris) (1966), 1(5/6), 221-54
SO
     CODEN: ANCPAC
DT
     Journal
     French
LΑ
IT
     14174-20-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
RN
     14174-20-0 CAPLUS
     Acetanilide, 2-[N-(3,4-dimethoxyphenethyl)benzamido]-2-phenyl- (8CI)
CN
     INDEX NAME)
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=> log y COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 40.12 180.99

FULL ESTIMATED COST

STN INTERNATIONAL LOGOFF AT 14:23:35 ON 15 MAY 2002

Welcome to STN International! Enter x:x

LOGINID:ssspta1611bxv

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

Welcome to STN International Web Page URLs for STN Seminar Schedule - N. America NEWS 1 NEWS 2 Jan 25 BLAST(R) searching in REGISTRY available in STN on the Web NEWS 3 FSTA has been reloaded and moves to weekly updates

NEWS 4 Feb 01 DKILIT now produced by FIZ Karlsruhe and has a new update frequency

Feb 19 Access via Tymnet and SprintNet Eliminated Effective 3/31/02 NEWS 5

NEWS 6 Mar 08 Gene Names now available in BIOSIS NEWS 7 Mar 22 TOXLIT no longer available

NEWS 8 Mar 22 TRCTHERMO no longer available

NEWS 9 Mar 28 US Provisional Priorities searched with P in CA/CAplus and USPATFULL

NEWS 10 Mar 28 LIPINSKI/CALC added for property searching in REGISTRY
NEWS 11 Apr 02 PAPERCHEM no longer available on STN. Use PAPERCHEM2 instead.
NEWS 12 Apr 08 "Ask CAS" for self-help around the clock
NEWS 13 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 14 Apr 09 ZDB will be removed from STN
NEWS 15 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 16 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS

NEWS 17 Apr 22 BIOSIS Gene Names now available in TOXCENTER

NEWS 18 Apr 22 Federal Research in Progress (FEDRIP) now available

NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d, CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP), AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002

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FILE 'HOME' ENTERED AT 14:02:57 ON 15 MAY 2002

=> ile reg ILE IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 14:03:07 ON 15 MAY 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 13 MAY 2002 HIGHEST RN 415678-09-0 DICTIONARY FILE UPDATES: 13 MAY 2002 HIGHEST RN 415678-09-0

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

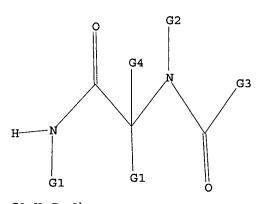
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Cy, Ak

G2 Cy,Ak

G3 Cb,Ak

G4 H,Me

Structure attributes must be viewed using STN Express query preparation.

09/810,648

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2.4% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

45 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS: PROJECTED ANSWERS:

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34653 TO 39827

L2

45 SEA SSS SAM L1

=> d scan

REGISTRY COPYRIGHT 2002 ACS L2 45 ANSWERS

L-Valinamide, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-L-.alpha.-glutamyl-N-IN methylglycyl-N-methyl-L-leucyl-L-valyl-N-methyl-L-leucyl-L-alanyl-D-alanyl-N-methyl-L-leucyl-N-methyl-L-leucyl-N-[2-hydroxy-1-(methoxycarbonyl)-3methyl-5-heptenyl]-N, N2-dimethyl-, [1S-(1R*,2S*,3S*,5E)]-(9CI)

SQL 11

MF C79 H125 N11 O17

Absolute stereochemistry. Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):44

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-cyclopropyl-3,4dihydro-3-[4-(methylthio)phenyl]-1-oxo-4-(1-pyrrolidinylcarbonyl)- (9CI)

MF C29 H34 N4 O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl)cyclopropylamino]carbonyl]phenyl]methyl]-3-[1,1'-biphenyl]-4-yl1,2,3,4-tetrahydro-1-oxo-N,N-bis(3-pyridinylmethyl)- (9CI)

MF C47 H42 N6 O4

PAGE 1-A

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2

L-Valinamide, N-[(1,1-dimethylethoxy)carbonyl]-O-methyl-L-tyrosyl-N-[2-hydroxy-4-[(3-methylbutyl)amino]-1-(2-methylpropyl)-4-oxobutyl]-N2-methyl-, [S-(R*,R*)]- (9CI)
C34 H58 N4 O7 IN

MF

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C32 H38 N6 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-1-oxo-Npropyl-3-(2-quinolinyl)-7-[(2,3,5,6-tetrafluoro-4-methylbenzoyl)amino](9CI)

MF C34 H31 F4 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 3,6,9,12,15,18,21,24,27,30,33,36,39,42,45-Pentadecaazaheptatetracosanamide
, 45-(2-aminoethyl)-47-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-

3,9,15,21,27,33,39-heptakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-7,13,19,25,31,37,43,46-octaoxo- (9CI)
MF C88 H115 N33 O32

PAGE 1-A

Me NH

$$CH_2$$
 $C = 0$
 $N - CH_2 - C - NH_2$
 CH_2
 CH_2

PAGE 1-B

PAGE 1-C

PAGE 2-C

PAGE 1-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-(3-carboxy-1-oxopropyl)-N-methylglycylglycyl-L-valyl-D-isoleucyl-L-threonyl-L-glutaminyl-L-isoleucyl-L-arginyl-L-prolyl- (9CI)

SQL 10

MF C49 H85 N15 O15

Absolute stereochemistry.

Me

HN

R

R

Et

NH

O

Ó

PAGE 1-B

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-(2-amino-2-oxoethyl)-N-[3-(diethylamino)propyl]-4-[[3,4-dihydro-1-oxo-7-[(1-oxo-3-butenyl)amino]-3-(2-pyridinyl)-2(1H)-isoquinolinyl]methyl]- (9CI)

MF C35 H42 N6 O4

$$\begin{array}{c} O & CH_2-C-NH_2 \\ O & CH_2-C-NH_2 \\ C-N-(CH_2)_3-NEt_2 \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Dermorphin, 2-D-arginine-4-(N-methylglycine)- (9CI)

SQL 7

MF C44 H59 N11 O10

PAGE 1-B

__OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C37 H31 F2 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Methioninamide, L-leucyl-N2-methyl-, monohydrochloride (9CI)

MF C12 H25 N3 O2 S . Cl H

HCl

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzeneacetamide, .alpha.-[benzoyl(phenylmethyl)amino]-N-(1,1dimethylethyl)- (9CI)

MF C26 H28 N2 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl)(2-methoxyethyl)amino]carbonyl]phenyl]methyl]-N-[(2-chlorophenyl)methyl]1,2,3,4-tetrahydro-3-(2-methoxyphenyl)-1-oxo-(9CI)

MF C37 H37 Cl N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Glycine, 2-cyclohexyl-N-[(1,1-dimethylethoxy)carbonyl]glycyl-N-methyl-3(methylsulfonyl)-L-alanyl-3-amino-2-hydroxyhexanoylglycyl-2-phenyl-,
1,1-dimethylethyl ester, (2S)- (9CI)

SQL 5
MF C38 H61 N5 O11 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN D-Alaninamide, N-[(tetrahydro-2-furanyl)carbonyl]glycyl-3-(2-naphthalenyl) D-alanyl-4-chloro-D-phenylalanyl-3-(3-pyridinyl)-D-alanyl-L-seryl-N-methyl L-tyrosyl-N6-(3-pyridinyl)carbonyl)-L-lysyl-L-leucyl-N6-(1-methylethyl)-L lysyl-L-prolyl-, (S)- (9CI)
SQL 11
MF C85 H111 Cl N16 O16
CI COM

PAGE 1-A

O ||
H₂N-C-CH-NH-C------| ||
Me O

PAGE 1-B

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-3-(6methyl-2-pyridinyl)-1-oxo-N-2-propenyl-4-(1-pyrrolidinylcarbonyl)- (9CI) MF C28 H33 N5 O4

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{C} \\ \text{O} \\ \text{N} \\ \text{C} \\ \text$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-(3-ethoxypropyl)-3,4-dihydro-1-oxo-4-(1-pyrrolidinylcarbonyl)-3-(2-quinolinyl)- (9CI)

MF C33 H39 N5 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 7-Oxa-2,5,10,13-tetraazatetradecan-14-oic acid, 10-[2-[[1-(cyclohexylmethyl)-2-hydroxy-5-methylhexyl]amino]-1-(1H-imidazol-4-ylmethyl)-2-oxoethyl]-2,5-dimethyl-1-(4-morpholinyl)-1,6,9-trioxo-8-(phenylmethyl)-, phenylmethyl ester, [1S-[1R*[R*(R*)],2R*]]- (9CI)

MF C49 H72 N8 O9

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

PAGE 1-B

PAGE 1-A

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-7-[(2-fluorobenzoyl)amino]-3,4-dihydro-1-oxo-N-propyl-3-(2-quinolinyl)- (9CI)

MF C33 H32 F N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN L-Leucine, N-[N-[N-[N-[N-[3-(3,4-dihydroxyphenyl)-1-oxopropyl]-N-methyl-L-

valyl]-L-isoleucyl]-L-asparaginyl]-L-.alpha.-aspartyl]- (9CI)
SQL 5
MF C35 H54 N6 O12

Absolute stereochemistry.

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C22 H32 N4 O2 . x C2 H F3 O2

CM 1

Absolute stereochemistry.

CM 2

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3-(3,4-difluorophenyl)-3,4-dihydro-7[(methoxyacetyl)amino]-1-oxo-2(1H)-isoquinolinyl]methyl]-N-(2methoxyethyl)- (9CI)

MF C31 H32 F2 N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alanine, N-[N-acetyl-N-methyl-3-(1-pyrenyl)-D-alanyl]-3-(1-pyrenyl)-,
 methyl ester (9CI)

MF C42 H34 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Phenylalaninamide, N-[(2E)-4-(1-aminocyclobutyl)-1-oxo-2-butenyl]-Nmethyl-3-(2-naphthalenyl)-D-alanyl-N,N.alpha.-dimethyl- (9CI)

MF C33 H40 N4 O3

Absolute stereochemistry.
Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

SQL 4

MF C30 H41 N7 O9 S

CI COM

Absolute stereochemistry.

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-O-(1,1dimethylethyl)-N-methyl-L-tyrosyl-D-alanylglycyl-N-[1-(hydroxymethyl)-3(methylthio)propyl]-N.alpha.-propyl-, (S)- (9CI)

SQL 5

MF C41 H63 N5 O8 S

PAGE 1-A

CH2-Ph

O Me

| O CH2-OH

| | | |

t-BuO-C-N O Me O O CH-C-NH-CH-CH2
CH2-CH-C-NH-CH-C-NH-CH2-C-N-Pr-n

PAGE 1-B

- CH₂-SMe

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Serine, 4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-N-[[(4-methoxyphenyl)methoxy]carbonyl]-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-, methyl ester (9CI)

SQL 12

MF C82 H108 N24 O34

PAGE 2-B

PAGE 3-A

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-3-(2-methoxyphenyl)-1-oxo-N-[2-(2-pyridinyl)ethyl]-4-[[[[4-(trifluoromethyl)phenyl]methyl]amino]carbonyl]- (9CI)

MF C37 H36 F3 N5 O5

PAGE 1-A

$$\begin{array}{c} \text{CF}_3 \\ \text{CH}_2 \\ \text{NH} \\ \text{C} \\ \text{CH}_2 - \text{CH}_2 - \text{N} - \text{C} - \text{CH}_2 - \text{CH}_2 - \text{N} \\ \text{N} \\ \text{H}_2 \text{N} - \text{C} - \text{CH}_2 \\ \text{O} \end{array}$$

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Leucine, N-[(2S)-4-methyl-1-oxo-2-[(2R)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropoxy]pentyl]-L-valyl-N-methyl-L-leucyl-L-phenylalanyl-, methyl ester (9CI)

SQL 4

MF C44 H63 F3 N4 O9

Absolute stereochemistry.

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Valine, N-[N-[N-[(2-chlorophenyl)acetyl]-N-[2-[methyl[(3-methylphenyl)methyl]amino]ethyl]-L-leucyl]-3-(1-naphthalenyl)-D-alanyl]-,
methyl ester (9CI)

MF C44 H55 Cl N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-4-[[(2-chlorophenyl)methyl]amino]carbonyl]-3,4-dihydro-3-[4-(methylthio)phenyl]-1-oxo-N-(3-pyridinylmethyl)- (9CI)

MF C35 H34 C1 N5 O4 S

PAGE 1-A

$$\begin{array}{c|c} & & & & \\ & & & & \\ & & & & \\ & & & \\ H_2N-C-CH_2 & & & \\ & & & \\ N & & & \\ & & & \\ CH_2-N-C-CH_2-CH_2-N & \\ & & & \\ & & & \\ \end{array}$$

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl) (phenylmethyl) amino] carbonyl] phenyl] methyl] -1,2,3,4-tetrahydro-3-(4-hydroxyphenyl) -1-oxo-N-[[4-(trifluoromethyl) phenyl] methyl] - (9CI)
MF C41 H35 F3 N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN L-Valine, N-[N-[N-[5-(1H-imidazol-1-yl)-1-oxopentyl]-N-methylglycyl]-L.alpha.-aspartyl]-, mono(trifluoroacetate) (9CI)
SQL 4
MF C20 H31 N5 O7 . C2 H F3 O2
CM 1

$$(CH_2)_4$$
 Me
 O
 H
 CO_2H
 CO_2H
 CO_2H
 H
 CO_2H
 CO_2H

CM 2

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Phenylalanine, N2-(cyclohexylcarbonyl)-N6-[(1,1-dimethylethoxy)carbonyl]D-lysyl-N-methyl-D-phenylalanyl-4-chloro- (9CI)

MF C37 H51 Cl N4 O7

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3,4-dihydro-7-[(3-methoxy-1-oxopropyl)amino]-3-[4-(methylthio)phenyl]-1-oxo-2(1H)-isoquinolinyl]methyl]-N-[2-(2-pyridinyl)ethyl]- (9CI)

MF C37 H39 N5 O5 S

PAGE 1-A

PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Histidinamide, N-[3-hydroxy-2-(hydroxymethyl)-2-methyl-1-oxopropyl]-Lphenylalanyl-N-[2-hydroxy-5-methyl-1-(2-methylpropyl)-4-[[[2-methyl-1-[[(2pyridinylmethyl)amino]carbonyl]butyl]amino]carbonyl]hexyl]-N.alpha.-methyl(9CI)

SQL 5

MF C45 H68 N8 O8

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Glutamic acid, N-[(8.xi.)-2,6-anhydro-1,7,8,9-tetradeoxy-9-oxo-9-[(2-phenylethyl)amino]-L-glycero-D-galacto-nonitol-8-yl]-N-[1-oxo-3-[4-(4-phenoxyphenoxy)phenyl]propyl]glycyl- (9CI)

MF C45 H51 N3 O13

Absolute stereochemistry.

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3-(3-cyanophenyl)-7-[(3,4-difluorobenzoyl)amino]-N-(3-ethoxypropyl)-3,4-dihydro-1-oxo-(9CI)

MF C33 H33 F2 N5 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-acetyl-3-(2-naphthalenyl)-D-alanyl-4-chloro-D phenylalanyl-6-nitro-D-tryptophyl-L-2,4-diaminobutanoyl-L-tyrosyl-D-lysyl L-arginyl-L-arginyl-N2-acetyl-L-arginyl-L-norleucyl-L-arginyl-L-prolyl (9CI)

SQL 13

MF C94 H135 Cl N30 O18

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Glycinamide, N-[2-(4-methoxyphenyl)ethyl]glycyl-N-hexylglycyl-N2-[1,1'-biphenyl]-4-yl- (9CI)

MF C33 H42 N4 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C32 H36 N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]glycyl-N.alpha.-ethyl4-fluoro- (9CI)

MF C18 H26 F N3 O4

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> log y COST IN U.S. DOLLARS

FULL ESTIMATED COST 0.76 0.97

SINCE FILE

TOTAL

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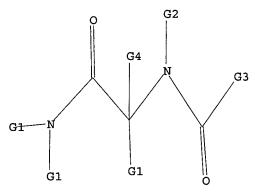
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L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Cy, Ak

G2 Cy,Ak

G3 Cb,Ak

G4 H, Me

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam SAMPLE SEARCH INITIATED 13:03:41 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 41378 TO ITERATE

2.4% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

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PROJECTED ITERATIONS:

815485 TO 839635

PROJECTED ANSWERS:

37850 TO 43250

49 ANSWERS

L2

49 SEA SSS SAM L1

=> d scan

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-3-(6-methyl-2-pyridinyl)-1-oxo-N-2-propenyl-4-(1-pyrrolidinylcarbonyl)- (9CI)

MF C28 H33 N5 O4

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{C} \\ \text{O} \\ \text{N} \\ \text{C} \\ \text{O} \\ \text$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):48

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Valinamide, N-[(1,1-dimethylethoxy)carbonyl]-O-methyl-L-tyrosyl-N-[2-hydroxy-4-[(3-methylbutyl)amino]-1-(2-methylpropyl)-4-oxobutyl]-N2-methyl, [S-(R*,R*)]- (9CI)

MF C34 H58 N4 O7

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2002 ACS L249 ANSWERS

2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-7-[(2-IN

fluorobenzoyl)amino]-3,4-dihydro-1-oxo-N-propyl-3-(2-quinolinyl)- (9CI)

MF C33 H32 F N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

49 ANSWERS REGISTRY COPYRIGHT 2002 ACS L2

IN .beta.-Alanine, N-[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]ph

enyl]acetyl]-N-(3-phenylpropyl)glycyl-N-(3-phenylpropyl)- (9CI)

MF C40 H46 N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alanine, N-[N-acetyl-N-methyl-3-(1-pyrenyl)-D-alanyl]-3-(1-pyrenyl)-,
 methyl ester (9CI)

MF C42 H34 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl) (2-methoxyethyl) amino] carbonyl]phenyl]methyl]-N-[(2-chlorophenyl)methyl]1,2,3,4-tetrahydro-3-(2-methoxyphenyl)-1-oxo- (9CI)
- MF C37 H37 Cl N4 06

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Valinamide, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-L-.alpha.-glutamyl-Nmethylglycyl-N-methyl-L-leucyl-L-valyl-N-methyl-L-leucyl-L-alanyl-D-alanylN-methyl-L-leucyl-N-methyl-L-leucyl-N-[2-hydroxy-1-(methoxycarbonyl)-3methyl-5-heptenyl]-N,N2-dimethyl-, [1S-(1R*,2S*,3S*,5E)]- (9CI)

SQL 11

MF C79 H125 N11 O17

Absolute stereochemistry.

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2 (1H) - Isoquinolinepropanamide, N-(2-amino-2-oxoethyl) -N-(3-ethoxypropyl) -

3,4-dihydro-1-oxo-4-(1-pyrrolidinylcarbonyl)-3-(2-quinolinyl)- (9CI)

MF C33 H39 N5 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-(3-carboxy-1-oxopropyl)-N-methylglycylglycyl-L-valyl-D-isoleucyl-L-threonyl-L-glutaminyl-L-isoleucyl-L-arginyl-L-prolyl- (9CI)

SQL 10

MF C49 H85 N15 O15

PAGE 1-A ÒН R Me HŅ ΗN Εt Мe HN HN N H Me NH₂ NH H₂N (CH₂)₃Мe NH NH_2

PAGE 1-B

49 ANSWERS REGISTRY COPYRIGHT 2002 ACS L-Leucine, N-[N-[N-[N-[3-(3,4-dihydroxyphenyl)-1-oxopropyl]-N-methyl-L-valyl]-L-isoleucyl]-L-asparaginyl]-L-alpha.-aspartyl]- (9CI) IN

SQL

C35 H54 N6 O12 MF

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C37 H31 F2 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzeneacetamide, .alpha.-[benzoyl(phenylmethyl)amino]-N-(1,1dimethylethyl)- (9CI)

MF C26 H28 N2 O2

$$\begin{array}{c|c} O & Ph & O \\ || & || & || \\ Ph-C-N-CH-C-NHBu-t \\ | & \\ Ph-CH_2 \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

SQL 5

MF C38 H61 N5 O11 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2 (dimethylamino)ethyl]-3,4-dihydro-3-(4-methylphenyl)-1-oxo-4-[[(3-pyridinylmethyl)amino]carbonyl]- (9CI)

MF C32 H38 N6 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN L-Valine, N-[N-[N-[5-(1H-imidazol-1-yl)-1-oxopentyl]-N-methylglycyl]-L.alpha.-aspartyl]-, mono(trifluoroacetate) (9CI)
SQL 4
MF C20 H31 N5 O7 . C2 H F3 O2
CM 1

Absolute stereochemistry.

$$(CH_2)_{4}$$

$$Me$$

$$O$$

$$H$$

$$CO_2H$$

$$CO_2H$$

$$CO_2H$$

$$CO_2H$$

$$CO_2H$$

$$CO_2H$$

$$CO_2H$$

$$CO_2H$$

$$CO_2H$$

CM 2

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzamide, N-(2-amino-2-oxoethyl)-N-[3-(diethylamino)propyl]-4-[[3,4-dihydro-1-oxo-7-[(1-oxo-3-butenyl)amino]-3-(2-pyridinyl)-2(1H)-isoquinolinyl]methyl]- (9CI)
MF C35 H42 N6 O4

$$\begin{array}{c} O \\ \parallel \\ O \\ CH_2-C-NH_2 \\ \parallel \\ C-N-(CH_2)_3-NEt_2 \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl](4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1oxopropyl]amino]cyclohexyl]- (9CI)

MF C38 H40 N4 O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Methioninamide, L-leucyl-N2-methyl-, monohydrochloride (9CI)

MF C12 H25 N3 O2 S . Cl H

HCl

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-cyclopropyl-3,4dihydro-3-[4-(methylthio)phenyl]-1-oxo-4-(1-pyrrolidinylcarbonyl)- (9CI)

MF C29 H34 N4 O4 S

$$\begin{array}{c|c} & & & & \\ & & & \\ & & \\ \text{MeS} & & \\ & & \\ \text{H}_2\text{N} & & \\ & &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN D-Valine, N-[N-[N-[(2-chlorophenyl)acetyl]-N-[2-[methyl[(3-methylphenyl)methyl]amino]ethyl]-L-leucyl]-3-(1-naphthalenyl)-D-alanyl]-,
 methyl ester (9CI)
MF C44 H55 Cl N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C34 H31 F4 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Phenylalanine, N-[(2E)-5-amino-5-methyl-1-oxo-2-hexenyl]-3-[1,1'-biphenyl]-4-yl-N-methyl-D-alanyl-N-methyl-, trimethylhydrazide (9CI)

MF C36 H47 N5 O3

Absolute stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Dermorphin, 2-D-arginine-4-(N-methylglycine) - (9CI)

SQL 7

MF C44 H59 N11 O10

PAGE 1-B

__OH

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C32 H36 N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Serine, 4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-N-[[(4-methoxyphenyl)methoxy]carbonyl]-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-, methyl ester (9CI)

SQL 12

MF C82 H108 N24 O34

PAGE 2-B

PAGE 3-A

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl)cyclopropylamino]carbonyl]phenyl]methyl]-3-[1,1'-biphenyl]-4-yl-1,2,3,4-tetrahydro-1-oxo-N,N-bis(3-pyridinylmethyl)- (9CI)

MF C47 H42 N6 O4

PAGE 1-A

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2002 ACS 49 ANSWERS L2

D-Phenylalanine, N2-(cyclohexylcarbonyl)-N6-[(1,1-dimethylethoxy)carbonyl]-IN D-lysyl-N-methyl-D-phenylalanyl-4-chloro- (9CI)

C37 H51 Cl N4 O7 MF

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2

49 ANSWERS REGISTRY COPYRIGHT 2002 ACS Glycinamide, N-[[(3-carboxyphenyl)amino]carbonyl]glycyl-N-methyl-N-phenyl-IN N2-8-quinolinyl- (9CI)

MF C28 H25 N5 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3-(3-cyanophenyl)-7-[(3,4-difluorobenzoyl)amino]-N-(3-ethoxypropyl)-3,4-dihydro-1-oxo-(9CI)

MF C33 H33 F2 N5 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Glycinamide, N-[2-(4-methoxyphenyl)ethyl]glycyl-N-hexylglycyl-N2-[1,1'-biphenyl]-4-yl- (9CI)

MF C33 H42 N4 O4

Ph
$$CH_2 - C - NH_2 O \\ | - C - CH_2 - N - C - CH_2 - NH - CH_2 - CH_2$$
O $(CH_2)_5 - Me$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]glycyl-N.alpha.-ethyl4-fluoro- (9CI)

MF C18 H26 F N3 O4

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-4-[[(2chlorophenyl)methyl]amino]carbonyl]-3,4-dihydro-3-[4-(methylthio)phenyl]-1oxo-N-(3-pyridinylmethyl)- (9CI)

MF C35 H34 Cl N5 O4 S

PAGE 1-A

$$\begin{array}{c|c} & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ H_2N-C-CH_2 & & \\ & & & \\$$

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 7-Oxa-2,5,10,13-tetraazatetradecan-14-oic acid, 10-[2-[[1-(cyclohexylmethyl)-2-hydroxy-5-methylhexyl]amino]-1-(1H-imidazol-4-ylmethyl)-2-oxoethyl]-2,5-dimethyl-1-(4-morpholinyl)-1,6,9-trioxo-8-(phenylmethyl)-, phenylmethyl ester, [1S-[1R*[R*(R*)],2R*]]- (9CI)

MF C49 H72 N8 O9

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3,4-dihydro-7-[(3-methoxy-1-oxopropyl)amino]-3-[4-(methylthio)phenyl]-1-oxo-2(1H)-isoquinolinyl]methyl]-N-[2-(2-pyridinyl)ethyl]- (9CI)

MF C37 H39 N5 O5 S

PAGE 1-A

O CH_2-C-NH_2 O CH_2-C-NH_2 MeO- $CH_2-CH_2-CH_2$ SMe

PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Glutamic acid, N-[(8.xi.)-2,6-anhydro-1,7,8,9-tetradeoxy-9-oxo-9-[(2-phenylethyl)amino]-L-glycero-D-galacto-nonitol-8-yl]-N-[1-oxo-3-[4-(4-phenoxyphenoxy)phenyl]propyl]glycyl- (9CI)

MF C45 H51 N3 O13

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-acetyl-3-(2-naphthalenyl)-D-alanyl-4-chloro-D phenylalanyl-6-nitro-D-tryptophyl-L-2,4-diaminobutanoyl-L-tyrosyl-D-lysyl L-arginyl-L-arginyl-N2-acetyl-L-arginyl-L-norleucyl-L-arginyl-L-prolyl (9CI)

SQL 13

MF C94 H135 Cl N30 O18

HN NH2

HN NH2

HN NH2

(CH2) 3

(CH2)

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2 (1H) -Isoquinolinepropanamide, N-(2-amino-2-oxoethyl) -3,4-dihydro-3-(2-methoxyphenyl) -1-oxo-N-[2-(2-pyridinyl)ethyl]-4-[[[[4-(trifluoromethyl)phenyl]methyl]amino]carbonyl]- (9CI)

MF C37 H36 F3 N5 O5

PAGE 1-A

PAGE 1-B

$$\begin{array}{c} \text{CF}_{3} \\ \text{CH}_{2} \\ \text{NH} \\ \text{C} \\ \text{C}$$

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-[(tetrahydro-2-furanyl)carbonyl]glycyl-3-(2-naphthalenyl)D-alanyl-4-chloro-D-phenylalanyl-3-(3-pyridinyl)-D-alanyl-L-seryl-N-methylL-tyrosyl-N6-(3-pyridinylcarbonyl)-L-lysyl-L-leucyl-N6-(1-methylethyl)-Llysyl-L-prolyl-, (S)- (9CI)

SQL 11

MF C85 H111 Cl N16 O16

CI COM

PAGE 1-A

PAGE 1-B

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl) (phenylmethyl) amino] carbonyl] phenyl] methyl] -1,2,3,4-tetrahydro-3-(4-hydroxyphenyl) -1-oxo-N-[[4-(trifluoromethyl) phenyl] methyl] - (9CI)
MF C41 H35 F3 N4 O5

$$\begin{array}{c} \text{CF}_3 \\ \text{CH}_2 \\ \text{NH} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{NH} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{O} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Ornithinamide, L-leucyl-N2-methyl-N-2-naphthalenyl-, trifluoroacetate (9CI)

MF C22 H32 N4 O2 . x C2 H F3 O2

CM 1

Absolute stereochemistry.

CM 2

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Histidinamide, N-[3-hydroxy-2-(hydroxymethyl)-2-methyl-1-oxopropyl]-Lphenylalanyl-N-[2-hydroxy-5-methyl-1-(2-methylpropyl)-4-[[[2-methyl-1-[[(2pyridinylmethyl)amino]carbonyl]butyl]amino]carbonyl]hexyl]-N.alpha.-methyl(9CI)

SQL 5

MF C45 H68 N8 O8

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

SQL 4

MF C30 H41 N7 O9 S

CI COM

Absolute stereochemistry.

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Glycinamide, N-[[(3-methylphenyl)amino]carbonyl]glycyl-N-methyl-N2-[3-[2-oxo-2-(phenylamino)ethoxy]phenyl]-N-phenyl- (9CI)

MF C33 H33 N5 O5

$$\begin{array}{c|c} & \circ & \text{Ph} \\ & \parallel & \parallel \\ & \text{CH}_2-\text{C-N-Me} \\ & \parallel \\ & \text{PhNH-C-CH}_2-\text{O} \\ & \parallel & \parallel \\ & \text{O} \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Leucine, N-[(2S)-4-methyl-1-oxo-2-[(2R)-3,3,3-trifluoro-2-methoxy-1-oxo2-phenylpropoxy]pentyl]-L-valyl-N-methyl-L-leucyl-L-phenylalanyl-, methyl
ester (9CI)

SQL 4

MF C44 H63 F3 N4 O9

Absolute stereochemistry.

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C55 H100 N12 O17 S2 Si

PAGE 1-A

PAGE 1-B

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 3,6,9,12,15,18,21,24,27,30,33,36,39,42,45-Pentadecaazaheptatetracosanamide
, 45-(2-aminoethyl)-47-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)3,9,15,21,27,33,39-heptakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)pyrimidinyl)acetyl]-7,13,19,25,31,37,43,46-octaoxo- (9CI)

MF C88 H115 N33 O32

PAGE 1-A

PAGE 1-B

PAGE 1-C

PAGE 2-C

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3-(3,4-difluorophenyl)-3,4-dihydro-7[(methoxyacetyl)amino]-1-oxo-2(1H)-isoquinolinyl]methyl]-N-(2methoxyethyl)- (9CI)

MF C31 H32 F2 N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Phenylalaninamide, N-[(2E)-4-(1-aminocyclobutyl)-1-oxo-2-butenyl]-N-methyl-3-(2-naphthalenyl)-D-alanyl-N,N.alpha.-dimethyl- (9CI)

MF C33 H40 N4 O3

Absolute stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-O-(1,1dimethylethyl)-N-methyl-L-tyrosyl-D-alanylglycyl-N-[1-(hydroxymethyl)-3(methylthio)propyl]-N.alpha.-propyl-, (S)- (9CI)

SQL 5

MF C41 H63 N5 O8 S

PAGE 1-A

PAGE 1-B

-- CH₂-- SMe

ALL ANSWERS HAVE BEEN SCANNED

=> log y COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL
ENTRY SESSION
0.76 0.97

STN INTERNATIONAL LOGOFF AT 13:04:40 ON 15 MAY 2002

Welcome to STN International! Enter x:x

LOGINID:ssspta1611bxv

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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FILE 'HOME' ENTERED AT 14:02:57 ON 15 MAY 2002

=> ile reg
ILE IS NOT A RECOGNIZED COMMAND

NEWS PHONE

NEWS WWW

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 14:03:07 ON 15 MAY 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 American Chemical Society (ACS)

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Please note that search-term pricing does apply when conducting SmartSELECT searches.

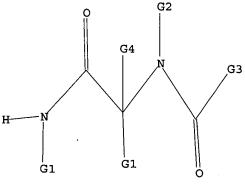
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> Uploading 09852965-2.str

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Cy, Ak

G2 Cy,Ak

G3 Cb,Ak

G4 H, Me

Structure attributes must be viewed using STN Express query preparation.

09/852,965

=> s l1 sss sam SAMPLE SEARCH INITIATED 14:03:36 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 41378 TO ITERATE

2.4% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01 45 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 815485 TO 839635 PROJECTED ANSWERS: 34653 TO 39827

L2 45 SEA SSS SAM L1

=> d scan

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Valinamide, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-L-.alpha.-glutamyl-Nmethylglycyl-N-methyl-L-leucyl-L-valyl-N-methyl-L-leucyl-L-alanyl-D-alanylN-methyl-L-leucyl-N-methyl-L-leucyl-N-[2-hydroxy-1-(methoxycarbonyl)-3methyl-5-heptenyl]-N,N2-dimethyl-, [1S-(1R*,2S*,3S*,5E)]- (9CI)

SQL 11 MF C79 H125 N11 O17

Absolute stereochemistry.

Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):44

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-cyclopropyl-3,4-dihydro-3-[4-(methylthio)phenyl]-1-oxo-4-(1-pyrrolidinylcarbonyl)- (9CI)

MF C29 H34 N4 O4 S

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ H_2N & & C - CH_2 \\ \hline & & & N - C - CH_2 - CH_2 - N \\ \hline & & & \\ & & & \\ & & & \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl)cyclopropylamino]carbonyl]phenyl]methyl]-3-[1,1'-biphenyl]-4-yl1,2,3,4-tetrahydro-1-oxo-N,N-bis(3-pyridinylmethyl)- (9CI)

MF C47 H42 N6 O4

PAGE 1-A

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Valinamide, N-[(1,1-dimethylethoxy)carbonyl]-O-methyl-L-tyrosyl-N-[2-hydroxy-4-[(3-methylbutyl)amino]-1-(2-methylpropyl)-4-oxobutyl]-N2-methyl-, [S-(R*,R*)]- (9CI)

MF C34 H58 N4 O7

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2 (dimethylamino)ethyl]-3,4-dihydro-3-(4-methylphenyl)-1-oxo-4-[[(3-pyridinylmethyl)amino]carbonyl]- (9CI)

MF C32 H38 N6 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-1-oxo-Npropyl-3-(2-quinolinyl)-7-[(2,3,5,6-tetrafluoro-4-methylbenzoyl)amino](9CI)

MF C34 H31 F4 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 3,6,9,12,15,18,21,24,27,30,33,36,39,42,45-Pentadecaazaheptatetracosanamide ,45-(2-aminoethyl)-47-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-

MF

3,9,15,21,27,33,39-heptakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-7,13,19,25,31,37,43,46-octaoxo- (9CI)
C88 H115 N33 O32

PAGE 1-A

Me NH

$$CH_2$$
 $C = 0$
 $N - CH_2 - C - NH_2$
 CH_2
 CH_2

PAGE 1-B

PAGE 1-C

PAGE 2-C

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

D-Alaninamide, N-(3-carboxy-1-oxopropyl)-N-methylglycylglycyl-L-valyl-D-IN isoleucyl-L-threonyl-L-glutaminyl-L-isoleucyl-L-arginyl-L-prolyl- (9CI)

SQL C49 H85 N15 O15

MF

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-(2-amino-2-oxoethyl)-N-[3-(diethylamino)propyl]-4-[[3,4-dihydro-1-oxo-7-[(1-oxo-3-butenyl)amino]-3-(2-pyridinyl)-2(1H)-isoquinolinyl]methyl]- (9CI)

MF C35 H42 N6 O4

$$\begin{array}{c} O \\ O \\ CH_2-C-NH_2 \\ O \\ C-N-(CH_2)_3-NEt_2 \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Dermorphin, 2-D-arginine-4-(N-methylglycine)- (9CI)

SQL 7

MF C44 H59 N11 O10

PAGE 1-B

__OH

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI)
MF C38 H40 N4 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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MF C37 H31 F2 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN L-Methioninamide, L-leucyl-N2-methyl-, monohydrochloride (9CI)

MF C12 H25 N3 O2 S . Cl H

● HCl

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzeneacetamide, .alpha.-[benzoyl(phenylmethyl)amino]-N-(1,1dimethylethyl)- (9CI)

MF C26 H28 N2 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl)(2-methoxyethyl)amino]carbonyl]phenyl]methyl]-N-[(2-chlorophenyl)methyl]-1,2,3,4-tetrahydro-3-(2-methoxyphenyl)-1-oxo-(9CI)

MF C37 H37 Cl N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

SQL 5

MF C38 H61 N5 O11 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-[(tetrahydro-2-furanyl)carbonyl]glycyl-3-(2-naphthalenyl)D-alanyl-4-chloro-D-phenylalanyl-3-(3-pyridinyl)-D-alanyl-L-seryl-N-methylL-tyrosyl-N6-(3-pyridinylcarbonyl)-L-lysyl-L-leucyl-N6-(1-methylethyl)-Llysyl-L-prolyl-, (S)- (9CI)

SQL 11

MF C85 H111 Cl N16 O16

CI COM

PAGE 1-B

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-3-(6-methyl-2-pyridinyl)-1-oxo-N-2-propenyl-4-(1-pyrrolidinylcarbonyl)- (9CI)

MF C28 H33 N5 O4

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{C} \\ \text{O} \\ \text{O} \\ \text{N} \\ \text{O} \\ \text$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-(3-ethoxypropyl)-3,4-dihydro-1-oxo-4-(1-pyrrolidinylcarbonyl)-3-(2-quinolinyl)- (9CI)

MF C33 H39 N5 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN L-Valine, N-[(1,1-dimethylethoxy)carbonyl]-3-[[[2(trimethylsilyl)ethoxy]carbonyl]amino]-D-alanyl-L-alanyl-S[(acetylamino)methyl]-N-methyl-L-cysteinyl-N-methyl-L-valyl-(2R)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-.beta.-alanyl-L-alanyl-S[(acetylamino)methyl]-N-methyl-L-cysteinyl-N-methyl-, methyl ester (9CI)
SQL 8
MF C55 H100 N12 O17 S2 Si

PAGE 1-A

PAGE 1-B

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-7-[(2-fluorobenzoyl)amino]-3,4-dihydro-1-oxo-N-propyl-3-(2-quinolinyl)- (9CI)
MF C33 H32 F N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Leucine, N-[N-[N-[N-[N-[3-(3,4-dihydroxyphenyl)-1-oxopropyl]-N-methyl-L-

09/852,965

valyl]-L-isoleucyl]-L-asparaginyl]-L-.alpha.-aspartyl]- (9CI)
SQL 5
MF C35 H54 N6 O12

Absolute stereochemistry.

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C22 H32 N4 O2 . \times C2 H F3 O2

CM 1

Absolute stereochemistry.

CM 2

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3-(3,4-difluorophenyl)-3,4-dihydro-7[(methoxyacetyl)amino]-1-oxo-2(1H)-isoquinolinyl]methyl]-N-(2methoxyethyl)- (9CI)

MF C31 H32 F2 N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alanine, N-[N-acetyl-N-methyl-3-(1-pyrenyl)-D-alanyl]-3-(1-pyrenyl)-,
methyl ester (9CI)

MF C42 H34 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Phenylalaninamide, N-[(2E)-4-(1-aminocyclobutyl)-1-oxo-2-butenyl]-N-methyl-3-(2-naphthalenyl)-D-alanyl-N,N.alpha.-dimethyl- (9CI)

MF C33 H40 N4 O3

Absolute stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

SQL 4

MF C30 H41 N7 O9 S

CI COM

Absolute stereochemistry.

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-O-(1,1dimethylethyl)-N-methyl-L-tyrosyl-D-alanylglycyl-N-[1-(hydroxymethyl)-3(methylthio)propyl]-N.alpha.-propyl-, (S)- (9CI)

SQL 5

MF C41 H63 N5 O8 S

PAGE 1-A

CH2-Ph

O Me

| O CH2-OH

| | | |

t-BuO-C-N O Me O O CH-C-NH-CH-CH-CH₂

CH2-CH-C-NH-CH-C-NH-CH₂

CH2-CH-C-NH-CH-C-NH-CH₂

t-BuO

PAGE 1-B

— СН₂— SМе

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Serine, 4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-N-[[(4-methoxyphenyl)methoxy]carbonyl]-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-, methyl ester (9CI)

SQL 12

MF C82 H108 N24 O34

PAGE 2-B

PAGE 3-A

L2

45 ANSWERS REGISTRY COPYRIGHT 2002 ACS 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-3-(2-IN methoxyphenyl)-1-oxo-N-[2-(2-pyridinyl)ethyl]-4-[[[[4-(trifluoromethyl)phenyl]methyl]amino]carbonyl]- (9CI)

C37 H36 F3 N5 O5 MF

PAGE 1-A

$$\begin{array}{c} \text{CF}_{3} \\ \text{CH}_{2} \\ \text{NH} \\ \text{C} \\ \text{C}_{2} \\ \text{N} \\ \text{C}_{2} \\ \text{C}_{3} \\ \text{CH}_{2} \\ \text{C}_{3} \\ \text{C}_{4} \\ \text{C}_{2} \\ \text{C}_{5} \\ \text{C}_{6} \\ \text{C}_{7} \\ \text$$

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Leucine, N-[(2S)-4-methyl-1-oxo-2-[(2R)-3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropoxy]pentyl]-L-valyl-N-methyl-L-leucyl-L-phenylalanyl-, methyl ester (9CI)

SQL 4

MF C44 H63 F3 N4 O9

Absolute stereochemistry.

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Valine, N-[N-[N-[(2-chlorophenyl)acetyl]-N-[2-[methyl](3methylphenyl)methyl]amino]ethyl]-L-leucyl]-3-(1-naphthalenyl)-D-alanyl]-,
methyl ester (9CI)

MF C44 H55 Cl N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-4-[[[(2-chlorophenyl)methyl]amino]carbonyl]-3,4-dihydro-3-[4-(methylthio)phenyl]-1-oxo-N-(3-pyridinylmethyl)- (9CI)

MF C35 H34 Cl N5 O4 S

PAGE 1-A

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl) (phenylmethyl) amino] carbonyl] phenyl]-methyl]-1,2,3,4-tetrahydro-3-(4-hydroxyphenyl)-1-oxo-N-[[4-(trifluoromethyl) phenyl] methyl]- (9CI)
MF C41 H35 F3 N4 O5

$$\begin{array}{c} CF_3 \\ CH_2 \\ NH \\ CH_2 \\ NH \\ CH_2 \\ CH_2 \\ CH_2 \\ NH \\ CH$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN L-Valine, N-[N-[N-[5-(1H-imidazol-1-yl)-1-oxopentyl]-N-methylglycyl]-L.alpha.-aspartyl]-, mono(trifluoroacetate) (9CI)
SQL 4
MF C20 H31 N5 O7 . C2 H F3 O2

Absolute stereochemistry.

1

CM

$$(CH_2)_4$$
 Me
 O
 H
 CO_2H
 CO_2H

CM 2

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Phenylalanine, N2-(cyclohexylcarbonyl)-N6-[(1,1-dimethylethoxy)carbonyl]D-lysyl-N-methyl-D-phenylalanyl-4-chloro- (9CI)

MF C37 H51 Cl N4 O7

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3,4-dihydro-7-[(3-methoxy-1-oxopropyl)amino]-3-[4-(methylthio)phenyl]-1-oxo-2(1H)isoquinolinyl]methyl]-N-[2-(2-pyridinyl)ethyl]- (9CI)

MF C37 H39 N5 O5 S

PAGE 1-A

PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Histidinamide, N-[3-hydroxy-2-(hydroxymethyl)-2-methyl-1-oxopropyl]-Lphenylalanyl-N-[2-hydroxy-5-methyl-1-(2-methylpropyl)-4-[[[2-methyl-1-[[(2pyridinylmethyl)amino]carbonyl]butyl]amino]carbonyl]hexyl]-N.alpha.-methyl(9CI)

SQL 5

MF C45 H68 N8 O8

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Glutamic acid, N-[(8.xi.)-2,6-anhydro-1,7,8,9-tetradeoxy-9-oxo-9-[(2-phenylethyl)amino]-L-glycero-D-galacto-nonitol-8-yl]-N-[1-oxo-3-[4-(4-phenoxyphenoxy)phenyl]propyl]glycyl- (9CI)

MF C45 H51 N3 O13

Absolute stereochemistry.

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3-(3-cyanophenyl)-7-[(3,4-difluorobenzoyl)amino]-N-(3-ethoxypropyl)-3,4-dihydro-1-oxo-(9CI)

MF C33 H33 F2 N5 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 45 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-acetyl-3-(2-naphthalenyl)-D-alanyl-4-chloro-Dphenylalanyl-6-nitro-D-tryptophyl-L-2,4-diaminobutanoyl-L-tyrosyl-D-lysylL-arginyl-L-arginyl-N2-acetyl-L-arginyl-L-norleucyl-L-arginyl-L-prolyl(9CI)

SQL 13

MF C94 H135 Cl N30 O18

REGISTRY COPYRIGHT 2002 ACS L2

45 ANSWERS REGISTRY COPYRIGHT 2002 ACS Glycinamide, N-[2-(4-methoxyphenyl)ethyl]glycyl-N-hexylglycyl-N2-[1,1'-IN biphenyl]-4-yl- (9CI) C33 H42 N4 O4

MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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MF C32 H36 N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]glycyl-N.alpha.-ethyl-4-fluoro-(9CI)

MF C18 H26 F N3 O4

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> log y COST IN U.S. DOLLARS

SINCE FILE ENTRY SESSION

TOTAL

FULL ESTIMATED COST

0.76

0.97

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NEWS 14 Apr 09 ZDB will be removed from STN
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ENTRY SESSION 0.21 0.21

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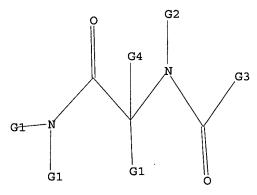
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> Uploading 09852965.str

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR



G1 H, Cy, Ak

G2 Cy,Ak

G3 Cb,Ak

G4 H, Me

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam SAMPLE SEARCH INITIATED 13:03:41 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 41378 TO ITERATE

2.4% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

PROJECTED ITERATIONS:

815485 TO 839635

49 ANSWERS

PROJECTED ANSWERS:

37850 TO 43250

L2

49 SEA SSS SAM L1

=> d scan

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IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-3-(6-methyl-2-pyridinyl)-1-oxo-N-2-propenyl-4-(1-pyrrolidinylcarbonyl)- (9CI)

MF C28 H33 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):48

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IN L-Valinamide, N-[(1,1-dimethylethoxy)carbonyl]-O-methyl-L-tyrosyl-N-[2-hydroxy-4-[(3-methylbutyl)amino]-1-(2-methylpropyl)-4-oxobutyl]-N2-methyl, [S-(R*,R*)]- (9CI)

MF C34 H58 N4 O7

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-7-[(2-fluorobenzoyl)amino]-3,4-dihydro-1-oxo-N-propyl-3-(2-quinolinyl)- (9CI)
- MF C33 H32 F N5 O4

$$\begin{array}{c|c} O & O & O & O \\ \hline C-NH & O & CH_2-C-NH_2 \\ \hline \\ F & O & CH_2-CH_2-C-N-Pr-n \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN .beta.-Alanine, N-[[3-methoxy-4-[[[(2-methylphenyl)amino]carbonyl]amino]ph enyl]acetyl]-N-(3-phenylpropyl)glycyl-N-(3-phenylpropyl)- (9CI)
- MF C40 H46 N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN D-Alanine, N-[N-acetyl-N-methyl-3-(1-pyrenyl)-D-alanyl]-3-(1-pyrenyl)-,
methyl ester (9CI)

MF C42 H34 N2 O4

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MF C37 H37 Cl N4 O6

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IN L-Valinamide, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-L-.alpha.-glutamyl-Nmethylglycyl-N-methyl-L-leucyl-L-valyl-N-methyl-L-leucyl-L-alanylN-methyl-L-leucyl-N-methyl-L-leucyl-N-[2-hydroxy-1-(methoxycarbonyl)-3methyl-5-heptenyl]-N,N2-dimethyl-, [1S-(1R*,2S*,3S*,5E)]- (9CI)

SQL 11

MF C79 H125 N11 O17

Absolute stereochemistry. Double bond geometry as shown.

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IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-(3-ethoxypropyl)-3,4-dihydro-1-oxo-4-(1-pyrrolidinylcarbonyl)-3-(2-quinolinyl)- (9CI)

MF C33 H39 N5 O5

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IN D-Alaninamide, N-(3-carboxy-1-oxopropyl)-N-methylglycylglycyl-L-valyl-D-isoleucyl-L-threonyl-L-glutaminyl-L-isoleucyl-L-arginyl-L-prolyl- (9CI)

SQL 10

MF C49 H85 N15 O15

PAGE 1-A ÒН R Me HŅ HN Εt Мe HN. H Me NH₂ NH H_2N (CH₂)₃Me NH NH₂

PAGE 1-B

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Leucine, N-[N-[N-[N-[N-[3-(3,4-dihydroxyphenyl)-1-oxopropyl]-N-methyl-L-valyl]-L-isoleucyl]-L-asparaginyl]-L-.alpha.-aspartyl]- (9CI)

SQL 5

MF C35 H54 N6 O12

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MF C37 H31 F2 N5 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Benzeneacetamide, .alpha.-[benzoyl(phenylmethyl)amino]-N-(1,1dimethylethyl)- (9CI)

MF C26 H28 N2 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Glycine, 2-cyclohexyl-N-[(1,1-dimethylethoxy)carbonyl]glycyl-N-methyl-3(methylsulfonyl)-L-alanyl-3-amino-2-hydroxyhexanoylglycyl-2-phenyl-,
1,1-dimethylethyl ester, (2S)- (9CI)

SQL 5

MF C38 H61 N5 O11 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-[2 (dimethylamino)ethyl]-3,4-dihydro-3-(4-methylphenyl)-1-oxo-4-[[(3-pyridinylmethyl)amino]carbonyl]- (9CI)

MF C32 H38 N6 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN L-Valine, N-[N-[N-[5-(1H-imidazol-1-yl)-1-oxopentyl]-N-methylglycyl]-L.alpha.-aspartyl]-, mono(trifluoroacetate) (9CI)

SQL 4

MF C20 H31 N5 O7 . C2 H F3 O2

CM 1

Absolute stereochemistry.

$$(CH_2)_{4}$$

$$Me$$

$$O$$

$$N$$

$$S$$

$$CO_2H$$

$$CO_2H$$

$$CO_2H$$

$$S$$

$$Pr-i$$

CM 2

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzamide, N-(2-amino-2-oxoethyl)-N-[3-(diethylamino)propyl]-4-[[3,4-dihydro-1-oxo-7-[(1-oxo-3-butenyl)amino]-3-(2-pyridinyl)-2(1H)-isoquinolinyl]methyl]- (9CI)
MF C35 H42 N6 O4

$$\begin{array}{c} O \\ \parallel \\ O \\ CH_2-C-NH_2 \\ \parallel \\ C-N-(CH_2)_3-NEt_2 \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1oxopropyl]amino]cyclohexyl]- (9CI)

MF C38 H40 N4 O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN L-Methioninamide, L-leucyl-N2-methyl-, monohydrochloride (9CI)

MF C12 H25 N3 O2 S . Cl H

● HCl

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IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-N-cyclopropyl-3,4-dihydro-3-[4-(methylthio)phenyl]-1-oxo-4-(1-pyrrolidinylcarbonyl)- (9CI)
MF C29 H34 N4 O4 S

$$\begin{array}{c|c} & & & \\ & & \\ & & \\ H_2N & & C - CH_2 \\ \hline & & N - C - CH_2 - CH_2 - N \\ \hline & & \\ & & \\ O \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN D-Valine, N-[N-[N-[(2-chlorophenyl)acetyl]-N-[2-[methyl[(3-methylphenyl)methyl]amino]ethyl]-L-leucyl]-3-(1-naphthalenyl)-D-alanyl]-,
 methyl ester (9CI)
MF C44 H55 Cl N4 O5

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2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-1-oxo-N-IN propyl-3-(2-quinolinyl)-7-[(2,3,5,6-tetrafluoro-4-methylbenzoyl)amino]-(9CI)

C34 H31 F4 N5 O4 MF

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IN D-Phenylalanine, N-[(2E)-5-amino-5-methyl-1-oxo-2-hexenyl]-3-[1,1'biphenyl]-4-yl-N-methyl-D-alanyl-N-methyl-, trimethylhydrazide (9CI)

C36 H47 N5 O3 MF

Absolute stereochemistry. Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Dermorphin, 2-D-arginine-4-(N-methylglycine)- (9CI)

SQL 7

MF C44 H59 N11 O10

PAGE 1-B

__OH

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C32 H36 N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN L-Serine, 4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-N-[[(4-methoxyphenyl)methoxy]carbonyl]-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-L-seryl-4-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-L-2-aminobutanoyl-N-methyl-, methyl ester (9CI)

SQL 12

MF C82 H108 N24 O34

PAGE 1-A

PAGE 2-B

PAGE 3-A

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl)cyclopropylamino]carbonyl]phenyl]methyl]-3-[1,1'-biphenyl]-4-yl-1,2,3,4-tetrahydro-1-oxo-N,N-bis(3-pyridinylmethyl)- (9CI)

MF C47 H42 N6 O4

PAGE 1-A

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D-Phenylalanine, N2-(cyclohexylcarbonyl)-N6-[(1,1-dimethylethoxy)carbonyl]-IN D-lysyl-N-methyl-D-phenylalanyl-4-chloro- (9CI)

C37 H51 Cl N4 O7 MF

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2

49 ANSWERS REGISTRY COPYRIGHT 2002 ACS Glycinamide, N-[[(3-carboxyphenyl)amino]carbonyl]glycyl-N-methyl-N-phenyl-IN

C28 H25 N5 O5 MF

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2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3-(3-cyanophenyl)-7-IN [(3,4-difluorobenzoyl)amino]-N-(3-ethoxypropyl)-3,4-dihydro-1-oxo- (9CI) MF C33 H33 F2 N5 O5

Eto-
$$(CH_2)_3$$
-N-C- CH_2 - CH_2

NH-C

 H_2N -C- CH_2

O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2

49 ANSWERS REGISTRY COPYRIGHT 2002 ACS Glycinamide, N-[2-(4-methoxyphenyl)ethyl]glycyl-N-hexylglycyl-N2-[1,1'-IN biphenyl]-4-yl- (9CI)

C33 H42 N4 O4 MF

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IN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]glycyl-N.alpha.-ethyl4-fluoro- (9CI)

MF C18 H26 F N3 O4

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

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IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-4-[[(2chlorophenyl)methyl]amino]carbonyl]-3,4-dihydro-3-[4-(methylthio)phenyl]-1oxo-N-(3-pyridinylmethyl)- (9CI)

MF C35 H34 Cl N5 O4 S

PAGE 1-A

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN 7-Oxa-2,5,10,13-tetraazatetradecan-14-oic acid, 10-[2-[[1-

(cyclohexylmethyl) -2-hydroxy-5-methylhexyl]amino]-1-(1H-imidazol-4-ylmethyl)-2-oxoethyl]-2,5-dimethyl-1-(4-morpholinyl)-1,6,9-trioxo-8-(phenylmethyl)-, phenylmethyl ester, [1S-[1R*[R*(R*)],2R*]]- (9CI)

MF C49 H72 N8 O9

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IN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3,4-dihydro-7-[(3-methoxy-1-oxopropyl)amino]-3-[4-(methylthio)phenyl]-1-oxo-2(1H)-isoquinolinyl]methyl]-N-[2-(2-pyridinyl)ethyl]- (9CI)

MF C37 H39 N5 O5 S

PAGE 1-A

O
CH₂-C-NH₂

O
CH₂-C-NH₂

MEO-CH₂-CH₂-CH₂

O
N-CH₂-CH₂-CH₂

PAGE 1-B



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IN L-Glutamic acid, N-[(8.xi.)-2,6-anhydro-1,7,8,9-tetradeoxy-9-oxo-9-[(2-phenylethyl)amino]-L-glycero-D-galacto-nonitol-8-yl]-N-[1-oxo-3-[4-(4-phenoxyphenoxy)phenyl]propyl]glycyl- (9CI)

MF C45 H51 N3 O13

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN D-Alaninamide, N-acetyl-3-(2-naphthalenyl)-D-alanyl-4-chloro-D phenylalanyl-6-nitro-D-tryptophyl-L-2,4-diaminobutanoyl-L-tyrosyl-D-lysyl L-arginyl-L-arginyl-N2-acetyl-L-arginyl-L-norleucyl-L-arginyl-L-prolyl (9CI)

SQL 13

MF C94 H135 Cl N30 O18

PAGE 1-B

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IN 2(1H)-Isoquinolinepropanamide, N-(2-amino-2-oxoethyl)-3,4-dihydro-3-(2-methoxyphenyl)-1-oxo-N-[2-(2-pyridinyl)ethyl]-4-[[[[4-(trifluoromethyl)phenyl]methyl]amino]carbonyl]- (9CI)

MF C37 H36 F3 N5 O5

PAGE 1-A

$$\begin{array}{c} \text{CF}_{3} \\ \text{CH}_{2} \\ \text{NH} \\ \text{C} \\ \text{C} \\ \text{C} \\ \text{O} \\ \text{C} \\ \text{C} \\ \text{O} \\ \text{O} \\ \text{C} \\ \text{O} \\ \text{O}$$

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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SQL 11

MF C85 H111 Cl N16 O16

CI COM

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PAGE 2-A

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IN 4-Isoquinolinecarboxamide, 2-[[4-[[(2-amino-2-oxoethyl) (phenylmethyl) amino] carbonyl] phenyl] methyl] -1,2,3,4-tetrahydro-3-(4-hydroxyphenyl) -1-oxo-N-[[4-(trifluoromethyl) phenyl] methyl] - (9CI)
MF C41 H35 F3 N4 O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN L-Ornithinamide, L-leucyl-N2-methyl-N-2-naphthalenyl-, trifluoroacetate (9CI)

MF C22 H32 N4 O2 . x C2 H F3 O2

CM 1

Absolute stereochemistry.

CM 2

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IN L-Histidinamide, N-[3-hydroxy-2-(hydroxymethyl)-2-methyl-1-oxopropyl]-Lphenylalanyl-N-[2-hydroxy-5-methyl-1-(2-methylpropyl)-4-[[[2-methyl-1-[[(2pyridinylmethyl)amino]carbonyl]butyl]amino]carbonyl]hexyl]-N.alpha.-methyl(9CI)

SQL 5

MF C45 H68 N8 O8

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

SQL 4

MF C30 H41 N7 O9 S

CI COM

Absolute stereochemistry.

L2 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Glycinamide, N-[[(3-methylphenyl)amino]carbonyl]glycyl-N-methyl-N2-[3-[2oxo-2-(phenylamino)ethoxy]phenyl]-N-phenyl- (9CI)

MF C33 H33 N5 05

$$\begin{array}{c|c} O & Ph \\ \parallel & \parallel \\ CH_2-C-N-Me \\ \parallel & \parallel \\ PhNH-C-CH_2-O \\ \hline \end{array}$$

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IN L-Leucine, N-[(2S)-4-methyl-1-oxo-2-[(2R)-3,3,3-trifluoro-2-methoxy-1-oxo2-phenylpropoxy]pentyl]-L-valyl-N-methyl-L-leucyl-L-phenylalanyl-, methyl
ester (9CI)

SQL 4

MF C44 H63 F3 N4 O9

Absolute stereochemistry.

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MF C55 H100 N12 O17 S2 Si

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

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IN 3,6,9,12,15,18,21,24,27,30,33,36,39,42,45-Pentadecaazaheptatetracosanamide
 , 45-(2-aminoethyl)-47-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl) 3,9,15,21,27,33,39-heptakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H) pyrimidinyl)acetyl]-7,13,19,25,31,37,43,46-octaoxo- (9CI)

MF C88 H115 N33 O32

PAGE 1-A

Me
$$NH$$
 CH_2
 $C=0$
 $N-CH_2-C-NH_2$
 CH_2
 NH
 CH_2
 NH
 $O=C$
 CH_2
 NH
 $O=C$
 CH_2

PAGE 1-B

PAGE 1-C

PAGE 2-A

PAGE 2-C

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Benzamide, N-(2-amino-2-oxoethyl)-4-[[3-(3,4-difluorophenyl)-3,4-dihydro-7[(methoxyacetyl)amino]-1-oxo-2(1H)-isoquinolinyl]methyl]-N-(2methoxyethyl)- (9CI)

MF C31 H32 F2 N4 O6

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN D-Phenylalaninamide, N-[(2E)-4-(1-aminocyclobutyl)-1-oxo-2-butenyl]-N-methyl-3-(2-naphthalenyl)-D-alanyl-N, N.alpha.-dimethyl- (9CI)

MF C33 H40 N4 O3

Absolute stereochemistry.

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN L-Phenylalaninamide, N-[(1,1-dimethylethoxy)carbonyl]-O-(1,1-dimethylethyl)-N-methyl-L-tyrosyl-D-alanylglycyl-N-[1-(hydroxymethyl)-3-(methylthio)propyl]-N.alpha.-propyl-, (S)- (9CI)

SQL 5

MF C41 H63 N5 O8 S

PAGE 1-A

PAGE 1-B

- CH $_2-$ SMe

ALL ANSWERS HAVE BEEN SCANNED

=> log y COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE ENTRY

TOTAL SESSION

0.76 0.97

STN INTERNATIONAL LOGOFF AT 13:04:40 ON 15 MAY 2002

L4ANSWER 12 OF 13 CAPLUS COPYRIGHT 2002 ACS ΑN 1970:477105 CAPLUS DN 73:77105 TΙ Preparation and properties of mesoionic oxazolones Bayer, Horst O.; Huisgen, Rolf; Knorr, Rudolf; Schaefer, Fred C. ΑU Inst. Org. Chem., Univ. Muenchen, Munich, Ger. CS SO Chem. Ber. (1970), 103(8), 2581-97 CODEN: CHBEAM DT Journal German LΑ IT 28544-59-4P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of) RN28544-59-4 CAPLUS

Benzamide, N-methyl-N-[.alpha.-(p-tolylcarbamoyl)benzyl]- (8CI) (CA INDEX

L4 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2002 ACS
AN 1967:2461 CAPLUS
DN 66:2461
TI 2,3,4,5-Tetrahydro-1H-3-benzazepin-1-ones and hexahydroimidazoisoquinolines
AU Hazebroucq, Georges
CS Pharm., Centrale Hop., Paris, Fr.
SO Ann. Chim. (Paris) (1966), 1(5/6), 221-54
CODEN: ANCPAC

CN

DT Journal

LA French

IT 14174-20-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 14174-20-0 CAPLUS

CN Acetanilide, 2-[N-(3,4-dimethoxyphenethyl)benzamido]-2-phenyl- (8CI) (CA INDEX NAME)